Minor II: CLL113 Numerical Methods in Chemical Engineering

Total Marks: 15 **Date: 10/10/16**

Please do not seek *any* clarification. Make suitable assumptions wherever necessary.

1. Determine all the values of a, b, c, d, e and f for which the following function is a cubic spline:

$$f(x) = \begin{cases} ax^2 + b(x-1)^3 & x \in [0,\,1]; \\ cx^2 + d & x \in [1,\,2]; \\ ex^2 + f(x-2)^3 & x \in [2,\,3]. \end{cases}$$

[3]

2. Consider the approximation to the following integration:

$$\int_{-1}^{1} f(x)\,dx \approx f(\alpha) + f(-\alpha).$$

For what value(s) of α, if any, will this formula be *exact* for the function $f(x)$ being all polynomials of the form $a + bx + cx^3 + dx^4$, where a, b, c and d are constants? [4]

3. For two non-linear algebraic equations: $f_1(x, y) = 0$ and $f_2(x, y) = 0$, the programming function "$core(f_1, f_2, x, y)$" returns the value of functions f_1 and f_2 for input values of x and y. Write an algorithm for Newton-Raphson technique to find the roots x and y starting with initial guess x_0 and y_0. Use central difference formula to construct the Jacobian matrix. The convergence condition should be based on relative (or normalized) error. Show only the important steps. [3]

4. Consider the data points:

x	0	1	2	4	5	6
$f(x)$	1	14	15	5	6	19

Using the Newton-divided difference method, obtain coefficients of 7^{th} degree polynomial $a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 + a_5x^5 + a_6x^6 + a_7x^7$ which passes through *all* the points and find $f(3)$. Find the derivative $f'(1)$ using any 2^{nd} order accurate formula. Give at least two reasons why this value of derivative is not in agreement with the $f'(1)$ calculated from the fitted polynomial (exact value). [2+1.5]

5. Answer briefly:
   (a) For fitting function values at n data point where n is very large, explain why cubic spline is preferable over single interpolating polynomial of either Lagrange or Newton type? [1]
   (b) Briefly explain why numerical differentiation is less accurate computationally as compared to numerical integration. [0.5]